An Optimized Runge-Kutta Method for the Numerical Solution of the Oscillatory Problems

Abstract: In this study, an optimized explicit Runge-Kutta (RK) method, which is based on a method of Dormand with six-stage and fifth algebraic order with FSAL property (see in [1]) denoted as ORK5 method is constructed. The proposed method solves first-order ordinary differential equations (ODEs) by first converting the second order ODEs to an equivalent first order. The new method has zero phase-lag, zero amplification error and zero first derivative of the phase-lag. Absolute stability of the new method is as well shown. The numerical experiments are carried out to show the efficiency of the derived method in comparison with other existing RK methods. We found that the new method is more efficient than the existing RK methods.

Keywords: Numerical analysis; Ordinary differential equation; Runge-Kutta method

1.0 Introduction

In this paper, we are dealing with the initial value problems (IVPs) of the form:

$$y'(x) = f(x, y), \qquad y(x_0) = y_0,$$

$$y'(x_0) = y'_0, \quad x \in [a,b] \tag{1}$$

where;

$$y(x) = [y_1(x), y_2(x), ..., y_s(x)]^T$$

$$f(x,y) = [f_1(x,y), f_2(x,y), ..., f_s(x,y)]^T$$

y_0 is a given vector of initial conditions and their solution is oscillatory. This type of problem occurs in various applied fields such as quantum mechanics, electronics, physical chemistry, molecular dynamics, astronomy, chemical physics and control engineering. In effect, Equation (1) can be solved using Runge-Kutta methods or multi-step methods. The solution of Equation (1) often shows a pronounced oscillatory behavior. In general, most problems with oscillatory or periodical behavior are second order or higher order. Hence, it is important to reduce the higher order problems to first-order problems in order to solve the ODEs in Equation (1). Several researchers have improved numerical methods for solving oscillatory problems based on the phase-fitted and amplification fitted properties. Simos and Vigo-Aguiar [2] constructed a modified phase-fitted RK method with phase-lag of order infinity for the numerical solution of periodic IVPs based on the fifth algebraic-order RK method of Dormand and Prince. Chen *et al*., [3] improved traditional RK methods by introducing frequency-depending weights in the update. With the phase-fitting and amplification-fitting conditions and algebraic order conditions, new practical RK integrators are obtained and two of the new methods have updates that are also phase-fitted and amplification-fitted. With the evolution of RK methods, Papadopoulos *et al*., [4] developed a new Runge-Kutta-Nyström (RKN) method for the numerical solution of the Schrödinger equation with phase-lag and amplification error of order infinity based on the fourth-order RKN method by Dormand, El-Mikkawy, and Prince. Meanwhile, Moo *et al*., [5] derived two new RKN methods for solving second-order differential equations with oscillatory solutions based on two existing RKN methods, a fourth-order three-stage Garcias RKN method and fifth-order four-stage Hairers RKN method. The derived methods both have two variable coefficients with zero amplification error (zero dissipative) and phase-lag of order infinity. In the last few years, Senu *et al*. [6] constructed zero dissipative explicit RK method for solving second-order ODEs with periodical solutions which has algebraic order three with dissipation of order infinity. Fawzi *et al*., [7-8] developed fourth-algebraic-order phase-fitted and amplification-fitted modified RK method and fourth-order seven-stage phase-fitted and amplification-fitted RK methods respectively. Recently, Ahmad *et al*., [9] constructed a phase-fitted and amplification-fitted two-derivative RK method of high algebraic order for the numerical solution of first-order Initial Value Problems (IVPs) which possesses oscillatory solutions. This paper is organized as follows: In section 2, the phase-lag properties of explicit RK method is presented. Derivation of the optimized RK method is given in section 3. Meanwhile in section 4, the analysis of the stability property is discussed. The numerical results, discussion, and conclusion are dealt with in sections 5 and 6 respectively.

2.0 Phase Lag Analysis of Runge-Kutta Method

We consider the *m*-stage explicit RK method of the form:

$$y_{n+1} = y_n + h\sum_{i=1}^{m} b_i k_i \tag{2}$$

$$k_i = f\left(x_n + c_i h, y_n + h\sum_{j=1}^{i-1} a_{ij} k_j\right) \quad ; \quad i = 1, \ldots, m \tag{3}$$

The method is said to be explicit when $a_{ij} = 0$ for $i \le j$ and implicit otherwise. The method in Equations (2) and (3) can be reduced into Butcher tableau form (see Table 1).

Table 1: *m*-stage explicit Runge-Kutta method

0					
c_2	a_{21}				
.	.				
.	.				
.	.				
c_m	a_{m1}	.	.	.	$a_{m,am-1}$
	b_1	.	.	.	b_m

To derive the new method based on phase lag analysis, we consider the following test equation based on [10]:

$$y' = ivy \qquad (4)$$

where v is real. Then we compare the theoretical solution and the numerical solution for this equation. By requiring that the solutions are in phase with maximal order in the step-size h, we derive the so-called dispersion relation. Applying the above method in Equations (2) and (3) to the test Equation (4), we obtain:

$$y_n = a_*^n y_0$$

with

$$a_* = A_m\left(H^2\right) + iHB_m H^2 \quad ; \quad H = vh \qquad (5)$$

The amplification factor is $a_* = a_*(H)$, and y_n denotes the approximation to $y(x_n)$. A comparison of Equation (5) with the solution of Equation (4) leads to the following definition of the dispersion or phase error or phase-lag and the amplification error.

Definition 2.1: An explicit *m*-stage RK, presented in Table 1 the quantities:

$$t(H) = H - \arg\left[a_*(H)\right] \quad ; \quad a(H) = 1 - |a_*(H)| \qquad (6)$$

are called the dispersion or phase error or phase-lag and the amplification error respectively.

If $t(H) = O\left(H^{r+1}\right)$, and $a(H) = O\left(H^{s+1}\right)$ then the method is said to be phase-lag order r and dissipative order s. [7]

From Equation (6), it follows that,

$$a(H) = 1 - \sqrt{\left[A_m^2\left(H^2\right) + H^2 B_m^2\left(H^2\right)\right]} \qquad (7)$$

Meanwhile, for the Runge-Kutta method given in Table 1, the following formula is used for the direct calculation of the phase-lag order r and the phase-lag constant q.

$$\tan(H) - H\left[\frac{B_m(H^2)}{A_m(H^2)}\right] = qH^{r+1} + O(H^{s+3}) \qquad (8)$$

The analysis of phase-fitted (dispersion of order infinity) and amplification-fitted (dissipation of order infinity) are based on dispersion and dissipation quantities that have discussed above. The RK method is phase-fitted and amplification-fitted if the following conditions hold:

$$t(H) = 0 \qquad \text{and} \qquad a(H) = 0 \qquad (9)$$

3.0 Construction of the New Runge-Kutta Methods

In this section, an optimized Runge-Kutta method will be derived, based on the fifth-order Runge-Kutta method with six-stage derived by [1], which is given in the tableau as follows (see Table 2). To achieve this, we set b_1, b_2 and b_3 as free coefficients while all other coefficients are the same as in Table 2, first we compute the polynomials A_m^2 and B_m^2 in terms of Runge-Kutta coefficients in Table 2. Then from these polynomials, we obtain the quantities $t(H)$ and $a(H)$ and by nullification of the phase-lag, amplification error and phase-lag's derivative.

Table 2: Runge-Kutta method of order five

0							
$\frac{1}{5}$	$\frac{1}{5}$						
$\frac{3}{10}$	$\frac{3}{40}$	$\frac{9}{40}$					
$\frac{4}{5}$	$\frac{44}{45}$	$-\frac{56}{15}$	$\frac{32}{9}$				
$\frac{8}{9}$	$\frac{19372}{6561}$	$-\frac{25360}{2187}$	$\frac{64448}{6561}$	$-\frac{212}{729}$			
1	$\frac{9017}{3168}$	$-\frac{355}{33}$	$\frac{46732}{5247}$	$\frac{49}{176}$	$-\frac{5103}{18656}$		
1	b_1	b_2	b_3	b_4	b_5	b_6	
	$\frac{35}{384}$	0	$\frac{500}{1113}$	$\frac{125}{192}$	$-\frac{2187}{6784}$	$\frac{11}{84}$	0

Hence, we obtain a system of three equations as follows:

$$a(H) = \left(1 - \frac{1}{600}H^4 + QH^2\right) + H^2\left(\frac{1}{120}H^4 + PH^2 + b_3 + b_1 + \frac{65479}{142464} + b_2\right)^2 - 1 = 0 \qquad (10)$$

$$t(H)=\tan(H)-H\left(\frac{1}{120}H^4+PH^2+b_3+b_1+\frac{65479}{142464}+b_2\right)\left(1-\frac{1}{600}h^6+\frac{1}{24}h^4+Qh^2\right)^{-1}=0 \tag{11}$$

$$\begin{aligned}t'(H)=&1+\left[\tan(H)\right]^2-\left(\frac{1}{120}H^4+PH^2+b_3+b_1+\frac{65479}{142464}+b_2\right)\\&\left(1-\frac{1}{600}H^6+\frac{1}{24}H^4+QH^2\right)^{-1}-H\left(\frac{1}{30}H^3+2PH\right)\\&\left(1-\frac{1}{600}H^6+\frac{1}{24}H^4+QH^2\right)^{-1}+H\left(\frac{1}{120}H^4+PH^2+b_3+b_1+\frac{65479}{142464}+b_2\right)\\&\left(-\frac{1}{100}H^5+\frac{1}{6}H^3+2QH\right)\left(1-\frac{1}{600}H^6+\frac{1}{24}H^4+QH^2\right)^{-2}\end{aligned} \tag{12}$$

where

$$P=-\frac{163}{1113}-\frac{9}{200}b_3 \quad \text{and} \quad Q=-\frac{3}{10}b_3-\frac{1}{5}b_2-\frac{271}{742}$$

Solving simultaneously the system of equations (10), (11) and (12), we obtain the coefficients b_1,b_2 and b_3 which are completely dependent on H where H is the product of the step-size h and the frequency v. The expressions for b_1,b_2 and b_3 are too complicated, hence we replaced by their Taylor series expansion and obtained the following expressions:

$$\begin{aligned}b_1&=\frac{35}{384}+\frac{643}{45360}H^4+\frac{62677}{16329600}H^6+\frac{5933}{4435200}H^8+\frac{50184187}{9340531200}H^{10}+\frac{2560520257}{11769069312000}H^{12}+\ldots\\b_2&=-\frac{601}{15120}H^4-\frac{1831}{217728}H^6-\frac{26041}{798330}H^8-\frac{328333}{249080832}H^{10}-\frac{83804419}{156920924160}H^{12}+\ldots\\b_3&=\frac{500}{1113}+\frac{29}{1134}H^4+\frac{451}{81648}H^6+\frac{2171}{997920}H^8+\frac{410413}{467026560}H^{10}+\frac{20951107}{58845346560}H^{12}+\ldots\end{aligned} \tag{13}$$

4.0 Stability of the new method

In this section, the linear stability of the method developed is analyzed. Consider to the test Equation (4) where $v>0$, the exact solution of this equation with initial value $y(x_0)=y_0$ satisfies

$$y(x_0+h)=R(H)y_0 \tag{14}$$

When applying Equations (2), (3) to (4):

$$y_{n+1} = R(H)\, y_0 \tag{15}$$

$$R(H) = 1 + Hb^T (I - HA)^{-1} e \tag{16}$$

where $e = (1,\ldots,1)^T$, $A = \left[a_{ij}\right]$ and $b^T = \left[b_1, b_2, b_3, \ldots, b_m\right]$. $R(H)$ is called the stability function of the method in Equation (3).

Definition 4.1: A Runge-Kutta method is said to be absolutely stable if $\forall H \in (-h, 0)$, $|R\left(\hat{H}\right)| < 1$. [7]

The stability polynomial of the ORK5 method is given as follows:

$$R(H) = 1 + H + \frac{1}{2}H^2 + \frac{1}{6}H^3 + \frac{1}{24}H^4 + \frac{1}{120}H^5 + \frac{1}{720}H^6 + \frac{53}{25200}H^7 - \frac{1}{40320}H^8 + \frac{907}{1814400}H^9 + \frac{1}{3628800}H^{10} + \frac{39073}{199584000}H^{11} - \frac{1}{479001600}H^{12} + \frac{2462483}{31135104000}H^{13} + \frac{1}{87178291200}H^{14} + \frac{9164119691}{57164050944000}H^{15} + \frac{11547559819}{266765571072000}H^{16} + \frac{11547559819}{1778437140480000}H^{17} \tag{17}$$

The comparison of the stability region of the ORK5 method up to H^i, where $i = 8,10,12$ and its original method is plotted in Figure 1. The stability interval of the original method is -306567892 and the stability interval of this method with the coefficients of H^8, H^{10}, H^{12} is -3.306570336. Observing from the stability regions plotted in Figure 1, our new method is absolutely stable since $\forall H \in (-3.3, 0)$, $|R(H)| < 1$. We however obtained the result using maple package.

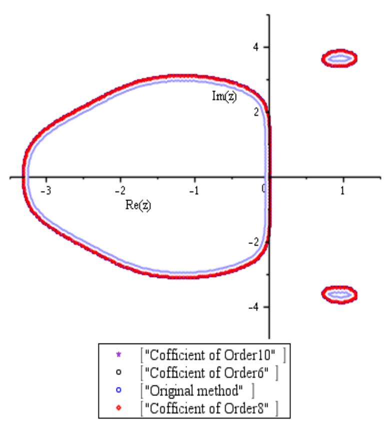

Figure 1: Stability region of ORK5 method for different order

4.1: Error Analysis

The local truncation error (LTE) of the new method is based on the Taylor series expansion of the differences y_{n+1} and $y(x_n+h)$.

$$LTE = y_{n+1} + y(x_n + h) \tag{18}$$

$$\begin{aligned}
LTE = {} & h^6\left[\frac{1}{3600}w^4 f_y f + \frac{2417}{381600} f_{xxxyy} f^2 + \frac{21361}{3052800} f_{xxxy} f_x + \frac{1517}{381600} f_{xxyyy} f^3\right] + \\
& h^6\left[\frac{35747}{6105600} f_{yxx} f_{xx} + \frac{239}{254400} f_{xyyyy} f^4 + \frac{30045211}{6328115200} f_{xyy} f_{xx} + \frac{17563}{9158400} f_{xy} f_{xxx}\right] + \\
& h^6\left[\frac{31}{8480} f_{xyy} f_x + \frac{1}{648000} f_{yyyyy} f^5 + \frac{2251}{4070400} f_y f_{xxxx} - \frac{1}{3600} f_{yyyy} f_x - \frac{1}{3600} f_{yyyyy} f\right] + \\
& h^6\left[\frac{61187}{3052800} ff_{xyy} f_y f_x + \frac{213825583}{32036083200} f_{xy} ff_{yy} f_x + \frac{22403}{3434400} f_{xy} f_{yy} f_y f^2\right] + \\
& h^6\left[\frac{17641}{10074240} ff_{yy} f_{yy} f_x + \frac{27}{13568} f^2 f_{yyy} f_y f_x + \frac{6859}{1526400} f_{xxxy} f\right] + \\
& h^6\left[\frac{14161}{1017600} ff_{xxyy} f_x + \frac{94}{11925} f_{xxxy} f_y f + \frac{17}{1272} f_{xxyy} f_y f^2 + \frac{343}{25440} f_{yxx} f_{xy} f\right] + \\
& h^6\left[\frac{349}{47700} f_{yxx} f_{yy} f^2 + \frac{2527}{190800} f_{yxx} f_y f_x + \frac{2527}{190800} f_{yxx} f_{yy} f + \frac{2317}{381600} f_{xyyy} f_y f^3\right] + \\
& h^6\left[\frac{7649}{1017600} ff_{xyy} f_{xx} + \frac{4979}{381600} f_{xyy} f_{xy} f^2 + \frac{113}{21200} f_{xyy} f_{yy} f^3 + \frac{11627}{763200} f_{xyy} f_{yy} f^2\right] + \\
& h^6\left[\frac{2257}{381600} f_{xyy} f_y f + \frac{833}{429300} f_{xy} f_{yyy} f^3 + \frac{431}{381600} f_{xy} f_y f_{xx} + \frac{333627097}{17085911040} ff_{yyy} f_{xx}\right] + \\
& h^6\left[\frac{217}{122112} ff_{yy} f_{xxx} + \frac{18649}{27475200} f^3 f_{yyy} f_x + \frac{1}{129600} f_{yyyy} f_y f^4 + \frac{104123}{54950400} f^2 f_{yyy} f_{xx}\right] + \\
& h^6\left[\frac{1}{64800} f_{yyy} f_{yy} f^4 - \frac{1}{43200} f_{yyy} f_{yy} f^3 + \frac{18649}{27475200} f^2 f_{yyy} f_x + \frac{1}{64800} f_{yyy} f_y f^3\right] + \\
& h^6\left[\frac{11}{43200} f_{yy} f_{yyy} f^2 + \frac{1252708019}{512577331200} f_{yy} f_{xx} f_x + \frac{75379}{50371200} f_{yy} f_y f_{xx} + \frac{73097}{6105600} f_{xxxxx}\right] + \\
& h^6\left[\frac{1}{3600} w^4 f_x + \frac{102427}{54950400} ff_{yy} f_y f_{xx} + \frac{2587}{339200} f^2 f_{xyyy} f_x\right] + O\left(h^7\right)
\end{aligned} \tag{19}$$

From Equation (19), it is clear that the order of the new method is five because all the terms of h lower than h^6 are vanished.

5.0 Tested problems and Numerical results

In this section, the performance of the proposed method ORK5 is compared with existing RK methods by considering the following problems. All problems below are tested using *C* code for solving differential equations where the solutions are periodic.

- ORK5: An optimized fifth-order RK method derived in this paper.
- MODRK5PLDPLAM: The phase-fitted six-stage fifth-order RK method derived in [11].
- MODPHARK5S: The modified phase-fitted fifth-order RK method given in [12].
- PHRK54: The higher order method of the phase-fitted embedded RK5(4) proposed in [13].
- RK-Fehlberg5th: An optimized fifth-order RK method derived in [14].

Problem 1: (Homogeneous Problem [15])

$$y_1' = y_2 \quad , \quad y_1(x) = 1$$

$$y_2' = -64y_1 \quad , \quad y_2(x) = -2$$

Theoretical solution:

$$y_1(x) = -\frac{1}{4}\sin(8x) + \cos(8x)$$

$$y_2(x) = -2\cos(8x) - 8\sin(8x)$$

Problem 2: (Inhomogeneous Problem [10])

$$y_1' = y_2 \quad , \quad y_1(x) = 1$$

$$y_2' = -v^2 y_1 + (v^2 - 1)\sin(x) \quad , \quad y_2(x) = v + 1$$

Estimated frequency: $v = 10$

Theoretical solution:

$$y_1(x) = \cos(vx) + \sin(vx) + \sin(x)$$

$$y_2(x) = -v\sin(vx) + v\cos(vx) + \cos(x)$$

Problem 3: (Almost periodic orbit problem [16])

$$y_1' = y_3 \quad , \quad y_1(x) = 1$$

$$y_3' = -y_1 + 0.001\cos(x) \quad , \quad y_3(x) = 0$$

$y_2' = y_4 \quad , \quad y_2(x) = 0$

$y_4' = -y_2 + 0.001\sin(x) \quad , \quad y_4(x) = 0.9995$

Theoretical solution:

$y_1(x) = \cos(x) + 0.0005x\sin(x)$

$y_2(x) = \sin(x) - 0.0005x\cos(x)$

$y_3(x) = -\sin(x) + 0.0005x\cos(x)$

$y_4(x) = \cos(x) + 0.0005x\sin(x)$

Problem 4: (Inhomogeneous system [17])

$y_1' = y_3 \quad , \quad y_1(x) = 1$

$y_2' = -13y_1 + 12y_2 + 9\cos(2x) - 12\sin(2x) \quad , \quad y_3(x) = -4$

$y_3' = y_4 \quad , \quad y_2(x) = 0$

$y_4' = 12y_1 - 13y_2 - 12\cos(2x) + 9\sin(2x) \quad , \quad y_4(x) = 8$

Estimated frequency: $v = 5$

Theoretical solution:

$y_1(x) = \sin(x) - \sin(5x) + \cos(2x)$

$y_2(x) = \sin(x) + \sin(5x) + \sin(2x)$

$y_3(x) = \cos(x) - 5\cos(5x) - 2\sin(2x)$

$y_4(x) = \cos(x) + 5\cos(5x) + 2\cos(2x)$

Problem 5: (Inhomogeneous system [18])

$y_1' = y_3 \quad , \quad y_1(x) = 0$

$y_2' = \frac{-101}{2} y_1 + \frac{99}{2} y_2 + \frac{93}{2}\cos(2x) - \frac{99}{2}\sin(2x) \quad , \quad y_3(x) = -10$

$y_3' = y_4 \quad , \quad y_2(x) = 1$

$$y_4' = \frac{99}{2} y_1 - \frac{101}{2} y_2 + \frac{93}{2} \sin(2x) - \frac{99}{2} \cos(2x) \quad , \quad y_3(x) = 12$$

Estimated frequency: $v = 10$

Theoretical solution:

$$y_1(x) = -\cos(10x) - \sin(10x) + \cos(2x)$$

$$y_2(x) = \cos(10x) + \sin(10x) + \cos(2x)$$

$$y_3(x) = 10\sin(10x) - 10\cos(10x) - 2\sin(2x)$$

$$y_4(x) = -10\sin(10x) + 10\cos(10x) + 2\cos(2x)$$

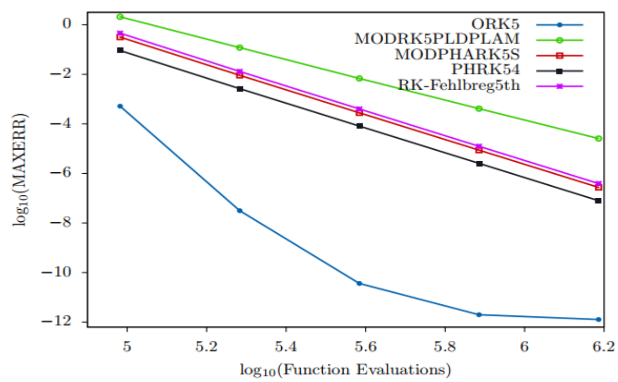

Figure 2: Comparison for ORK5, MODRK5PLDPLAM, MODPHARK5S, PHRK54 and RK-Fehlberg5th problem 1 with b=10000

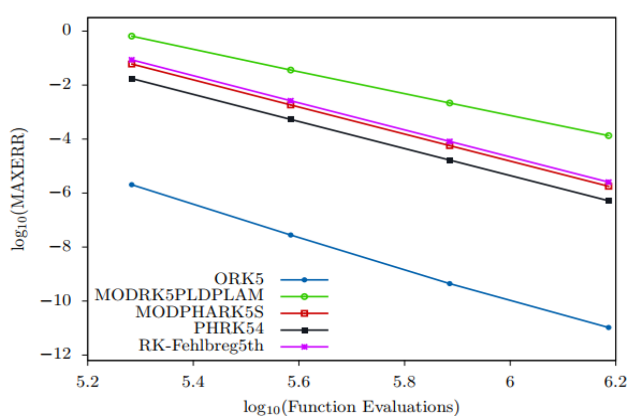

Figure 3: Comparison for ORK5, MODRK5PLDPLAM, MODPHARK5S, PHRK54 and RK-Fehlberg5th problem 2 with b=10000

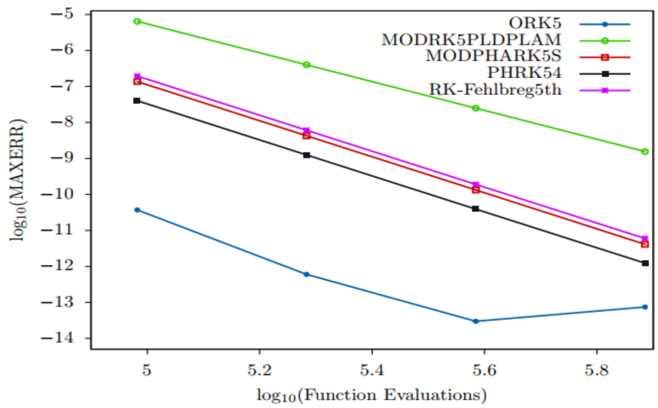

Figure 4: Comparison for ORK5, MODRK5PLDPLAM, MODPHARK5S, PHRK54 and RK-Fehlberg5th problem 3 with b=10000

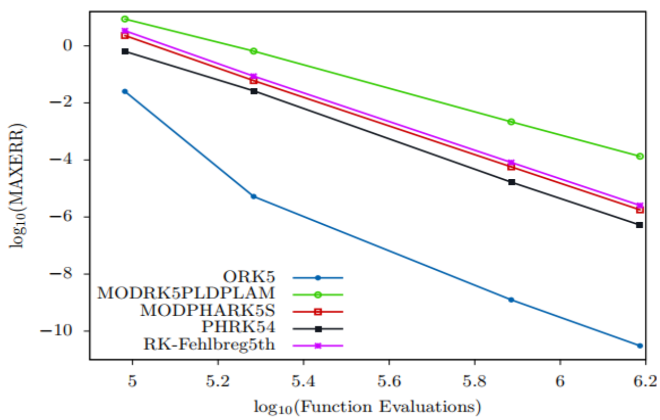

Figure 5: Comparison for ORK5, MODRK5PLDPLAM, MODPHARK5S, PHRK54 and RK-Fehlberg5th problem 4 with b=10000

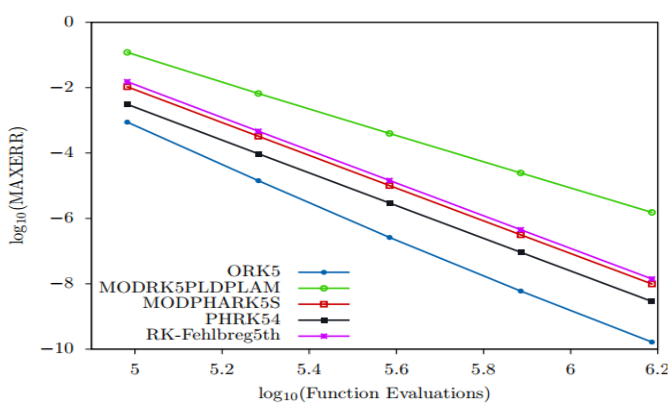

Figure 6: Comparison for ORK5, MODRK5PLDPLAM, MODPHARK5S, PHRK54 and RK-Fehlberg5th problem 5 with b=10000

6.0 Discussion and Conclusion

In this study, a six-stage fifth-order RK method denoted as ORK5 for solving first-order ODEs by first converting the second order ODEs to an equivalent first order with phase-lag and amplification error of order infinity and the first derivative of phase-lag is of order infinity is developed. The comparison is made with other well-known existing explicit RK methods that have same algebraic order which are found in [11-13] and [14]. In the numerical comparisons, we used the criteria based on computing the maximum error in the solution $\left[\max error = \max\left(|\, y\left(t_n - y_n\right)|\right)\right]$ which is equal to the maximum between absolute errors of the true solutions and the computed solutions. Figures 2-6 show the efficiency curves of Log10 (max error) against the computational effort measured by Log10 (function evaluations) required by each method and we observed that the new ORK5 method is more efficient for integration first-order differential equations possessing an oscillatory solution compared with other methods which are MODRK5PLDPLAM, MODPHARK5S, PHRK54 and RK-Fehlberg5th.

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